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A parametric symmetric linear four-step method for the efficient integration of the Schrödinger equation and related oscillatory problems

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ABSTRACT

In this article, we develop an explicit symmetric linear phase-fitted four-step method with a free coefficient as parameter. The parameter is used for the optimization of the method in order to solve efficiently the Schrödinger equation and related oscillatory problems. We evaluate the local truncation error and the interval of periodicity as functions of the parameter. We reveal a direct relationship between the periodicity interval and the local truncation error. We also measure the efficiency of the new method for a wide range of possible values of the parameter and compare it to other well known methods from the literature. The analysis and the numerical results help us to determine the optimal values of the parameter, which render the new method highly efficient.

1. Introduction

The numerical solution of the Schrödinger equation and related initial value problems with oscillatory/periodic solutions has attracted the interest of many researchers during the past decades [1–48]. We consider the one-dimensional time-independent Schrödinger equation, which is given by

$$y''(x) = \left(\frac{l(l+1)}{x^2} + V(x) - E\right) y(x) \tag{1}$$

where $\frac{l(l+1)}{x^2}$ is the *centrifugal potential*, with $x \in \mathcal{R}^*$ and $l = 0, 1, 2, \ldots$ expressing the principal angular momentum quantum number, $V(x)$ is the *potential*, E is the *energy* and $W(x) = \frac{l(l+1)}{x^2} + V(x)$ is the *effective potential*. We will consider a potential for which $\lim_{x\to\infty} V(x) = 0$ and therefore $\lim_{x\to\infty} W(x) = 0$.

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We consider $E > 0$ and divide $[x_{\min}, x_{\max}]$, where $x_{\min} < 0$ and $x_{\max} > 0$ are the boundaries of the integration interval and depend on the potential used, into subintervals $[a_i, b_i]$, where $a_i, b_i \in [x_{\min}, x_{\max}]$ (or $a_i, b_i \in [x_{\min}, -x_0) \cup (x_0, x_{\max}]$, when $l > 0$, where x_0 is chosen to be sufficiently close to 0 with the appropriate boundary conditions), so that on each subinterval $W(x)$ can be suitably approximated by a constant with value $\bar{W}_i$. The number of subintervals is equal to the number of steps performed during the integration. Then problem (1) can be expressed by the approximation

$$\begin{aligned} &y_i'' = (\bar{W}_i - E)\, y_i, \quad \text{whose solution is} \\ &y_i(x) = A_i\, e^{\sqrt{\bar{W}_i - E}\, x} + B_i\, e^{-\sqrt{\bar{W}_i - E}\, x}, \quad A_i,\ B_i\ \in \mathbb{R},\ \text{and } x \in [a_i, b_i]. \end{aligned} \tag{2}$$

We use the approach above, so that we can use an approximation $\bar{W}_i$ of the potential $W(x)$. This approximation is used in both the numerical integration and the local truncation error analysis of the method, when it is applied to the Schrödinger equation.

The majority of finite difference methods that are produced for the efficient solution of the above problem have no free parameters, which makes the systematic comparison and optimization of a certain family (or type) of methods difficult. This is more obvious during the construction of linear multistep methods, because not all parameters can be determined through conditions that are necessary for obtaining maximum algebraic/trigonometric order and/or other critical properties such as phase-fitting, minimum phase-lag etc. Some coefficients need to be selected so that the method has non-zero (or maximum) interval of stability/periodicity. However, the last task requires that the roots of the corresponding characteristic equation satisfy certain conditions, later described in the theory section. The procedure of selecting appropriate values can be performed analytically only in special cases and for small number of steps. Even when we find intervals that the coefficients must lie in, so that the interval of stability/periodicity is non-zero (or maximum), this is often not enough, because the efficiency of the method during the actual integration is of critical importance. The development, analysis and application of an algorithm with free coefficients can also reveal a desirable or an unwelcome property/behavior. We should finally note that this work should be considered as parameterizing a method or a family of methods and can be applied to different types of methods with various numbers of stages, different orders etc. This approach can in no way be inferior to the development of a single non-parametric method; instead it is a generalization that helps with the investigation of a whole family of methods.

In this work, we produce a parametric explicit symmetric linear four-step method with fourth algebraic order and zero phase-lag for the numerical solution of the above equation and related oscillatory problems.

More specifically, in Section 2, we provide the necessary definitions and theorems. In Section 3, we present the development, truncation error analysis and periodicity analysis of the method and also the direct relationship of the error to the periodicity interval. In Section 4, we show the application of the method to the Schrödinger equation and related problems and we measure its efficiency for a wide range of possible values of the parameter. We make a comparison to other methods in terms of efficiency and we provide the optimal values of the parameter. Finally in Section 5, we give some conclusions on the results of this work.

2. Theory

For the numerical solution of the initial value problem

$$y'' = f(x, y), \tag{3}$$

where f does not contain an explicit form of $y'(x)$, we define a multistep method of the form

$$\sum_{i=0}^{m} a_i y_{n+i} = h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}) \tag{4}$$

with m steps, which can be used over the equally spaced intervals $\{x_i\}_{i=0}^{m} \in [a, b]$ and $h = |x_{i+1} - x_i|,\ i = 0(1)m - 1$. The method is called symmetric if $a_i = a_{m-i}$ and $b_i = b_{m-i},\ i = 0(1)\lfloor \frac{m}{2} \rfloor$.

Method (4) is associated with the expression

$$L(x) = \sum_{i=0}^{m} a_i u(x + ih) - h^2 \sum_{i=0}^{m} b_i u''(x + ih) \tag{5}$$

where $u \in C^2$.

Definition 1. The multistep method (4) is said to be of algebraic order p if the associated expression L vanishes for any linear combination of the linearly independent functions $1, x, x^2, \ldots, x^{p+1}$.

2.1. Periodicity analysis of multistep methods

Here, we will provide the necessary definitions and theorems to perform a periodicity analysis of multistep methods [28]. We apply the linear m-step method (4) to the scalar test equation

$$y'' = -\omega^2 y, \quad \omega \in \mathcal{R}^+ \tag{6}$$

and then we solve the corresponding characteristic equation, which has m characteristic roots $\lambda_i,\ i = 0(1)m-1$, where λ_0 and λ_1 are the principal roots.

Definition 2 ([6]). If the characteristic roots satisfy the conditions $\lambda_0 = e^{I\phi(s)}$, $\lambda_1 = e^{-I\phi(s)}$, and $|\lambda_i| \leqslant 1,\ i = 2(1)m-1$ for all $s < s_0$, where $s = \omega h$ and $\phi(s)$ is a real function of s, then we say that the method has interval of periodicity $(0, s_0^2)$.

2.2. Phase-lag analysis of symmetric multistep methods

When a symmetric $2k$-step method is applied to the scalar test equation (6), a difference equation of the form

$$A_k(v)y_{n+k} + \cdots + A_1(v)y_{n+1} + A_0(v)y_n + A_1(v)y_{n-1} + \cdots + A_k(v)y_{n-k} = 0 \tag{7}$$

is obtained, where $v = \omega h$ and $A_0(v), A_1(v), \ldots, A_k(v)$ are polynomials in v, where $A_i(v) = a_i + b_i\, v^2,\ i = 0(1)k$.

The characteristic equation associated with (7) is

$$A_k(v)s^k + \cdots + A_1(v)s + A_0(v) + A_1(v)s^{-1} + \cdots + A_k(v)s^{-k} = 0. \tag{8}$$

Definition 3 ([27,25]). For any method corresponding to the characteristic equation (8), the phase-lag is defined as the term

$$t = v - \phi(v).$$

Then if the quantity $t = O(v^{q+1})$ as $v \to 0$, the order of phase-lag is q, where the characteristic roots are of the form $\lambda_0 = e^{I\phi(v)}$, $\lambda_1 = e^{-I\phi(v)}$, $v = \omega\, h$ and satisfy the conditions of Definition 2.

The following theorem provides a formula for the direct calculation of a linear multistep method.

Theorem 1 ([25]). *The symmetric $2k$-step method with characteristic equation given by (8) has phase-lag order q and phase-lag constant c given by*

$$\frac{2A_k(v)\cos(kv) + \cdots + 2A_j(v)\cos(jv) + \cdots + A_0(v)}{2k^2A_k(v) + \cdots + 2j^2A_j(v) + \cdots + 2A_1(v)} = -cv^{q+2} + O(v^{q+4}). \tag{9}$$

Definition 4. The multistep method (4) is called phase-fitted, when the phase-lag vanishes.

3. Development and analysis of the new parametric method

3.1. Development

We consider the explicit symmetric linear four-step method given below

$$y_2 + y_{-2} + a_1\,(y_1 + y_{-1}) + a_0\,y_0 = h^2\,(b_1(f_1 + f_{-1}) + b_0f_0)\,. \tag{10}$$

Our goal is to produce a phase-fitted method, that has a free coefficient as parameter. In this way, we will investigate the accuracy, local truncation and periodicity interval as functions of the parameter, in order to chose the optimal value.

The phase-lag (PL) of the above method, after following the procedure described in Section 2.2, is presented below

$$PL = \frac{4\,(\cos(v))^2 + \left(2\,b_1v^2 + 2\,a_1\right)\cos(v) + b_0v^2 - 2 + a_0}{8 + 2\,b_1v^2 + 2\,a_1}$$

where $v = \omega\, h$, ω is the dominant frequency of the problem and h is the step-length of integration.

In order that the above method has zero phase-lag along with the maximum algebraic order p, the following conditions must hold

$$PL = 0 \tag{11}$$

$$L(x^i) = 0, \quad i = 0, 1, \ldots, p+1. \tag{12}$$

For the aforementioned method, this leads to the solution below

$$\begin{aligned} a_0 &= -2 - 2\,a_1 \\ b_0 &= 4 + a_1 - 2\,b_1 \\ b_1 &= -\frac{4\,(\cos(v))^2 + 2\,\cos(v)a_1 + 4\,v^2 + v^2a_1 - 2\,a_1 - 4}{2\,v^2\,(\cos(v) - 1)} \end{aligned} \tag{13}$$

which renders the method of algebraic order four, as we will see in Section 3.2. We must note here that the method's coefficients depend on $v = \omega h$ and the free parameter a_1.

As $v \to 0$, both the numerator and the denominator tend to zero and the division of such numbers creates enormous round-off errors. In order to avoid such errors, we use their Taylor series expansions instead.

$$\begin{aligned} b_0 &= \frac{4}{3} + \frac{5}{6}a_1 + \left(-\frac{1}{120}a_1 + \frac{2}{15}\right)v^2 + \left(-\frac{13}{1890} - \frac{1}{3024}a_1\right)v^4 + \left(\frac{1}{18\,900} - \frac{1}{86\,400}a_1\right)v^6 \\ &+ \left(-\frac{13}{4\,989\,600} - \frac{1}{2\,661\,120}a_1\right)v^8 + \left(-\frac{691}{59\,439\,744\,000}a_1 - \frac{1559}{40\,864\,824\,000}\right)v^{10} \\ &+ \left(-\frac{47}{32\,691\,859\,200} - \frac{1}{2\,874\,009\,600}a_1\right)v^{12} + \left(-\frac{1}{24\,700\,515\,840} - \frac{3617}{355\,687\,428\,096\,000}a_1\right)v^{14} + \cdots \\ b_1 &= \frac{4}{3} + \frac{1}{12}a_1 + \left(\frac{1}{240}a_1 - \frac{1}{15}\right)v^2 + \left(\frac{13}{3780} + \frac{1}{6048}a_1\right)v^4 + \left(-\frac{1}{37\,800} + \frac{1}{172\,800}a_1\right)v^6 \\ &+ \left(\frac{13}{9\,979\,200} + \frac{1}{5\,322\,240}a_1\right)v^8 + \left(\frac{691}{118\,879\,488\,000}a_1 + \frac{1559}{81\,729\,648\,000}\right)v^{10} \\ &+ \left(\frac{47}{65\,383\,718\,400} + \frac{1}{5\,748\,019\,200}a_1\right)v^{12} + \left(\frac{1}{49\,401\,031\,680} + \frac{3617}{711\,374\,856\,192\,000}a_1\right)v^{14} + \cdots \end{aligned} \tag{14}$$

3.2. Local truncation error analysis

By substituting the coefficients from Eq. (14) to method (10), we obtain the principal term of the local truncation error for the general case of problem (3), which derives from the Taylor series expansion of the difference of the two sides of Eq. (10) and is given below

$$\mathrm{PLTE} = \frac{16 - a_1}{240}\left(y^{(6)}(x) + y^{(4)}(x)\omega^2\right)h^6. \tag{15}$$

Before making assumptions about the method's minimum error, we need first to consider the periodicity property.

We also present the term of the above expression for the case of the Schrödinger equation that contains the energy with the maximum power. This is derived via the application of the Schrödinger equation for the case described in Section 4.1.1, with $\omega = \sqrt{E - \bar{W}_i}$ and is provided below

$$\mathrm{PLTE}_{\mathrm{PF}} = \frac{16 - a_1}{240}h^6\left[\left(W(x) - \bar{W}_i\right)y(x)E^2 + \cdots\right].$$

We must note that in case $\omega = 0$ (classical, i.e. non-phase-fitted method) the term of the error with the maximum power of energy becomes

$$\mathrm{PLTE}_{\mathrm{CI}} = \frac{16 - a_1}{240}h^6\left[-y(x)E^3 + \cdots\right].$$

This reveals the importance of phase-fitting for the numerical integration of the Schrödinger equation, as the error decreases in comparison to the corresponding classical method.

3.3. Periodicity analysis

After applying method (10) with coefficients provided by (13) to the test problem $y'' = -\omega^2 y$, we compute the characteristic equation of Definition 2 for the new parametric method. The equation is provided by the expression below

$$\begin{aligned} &\lambda^4 + \frac{\left(2 - s^2a_1 - 2\cos(2s) - 4s^2\right)}{2\cos(s) - 2}\lambda^3 + \frac{\left(8\cos(s)s^2 + 4\cos(2s) - 4\cos(s) + 2s^2a_1\cos(s)\right)2\cos(s) - 2}{2\cos(s) - 2}\lambda^2 \\ &+ \frac{\left(2 - s^2a_1 - 2\cos(2s) - 4s^2\right)}{2\cos(s) - 2}\lambda + 1 = 0, \quad \text{where } s = \omega h. \end{aligned} \tag{16}$$

For a wide range of values of the coefficient a_1, we determine computationally the periodicity interval, by checking the conditions of Definition 2 for the set $\left\{\widehat{s} \mid \widehat{s}^2 \in (0, s_0^2)\right\}$, where $\widehat{s} = n\,\Delta s,\ n \in \mathbb{N}_0$ and $\Delta s = 10^{-3}$ and we present the results in Fig. 1.

We must note here that the method has a non-vanishing interval of periodicity only when $a_1 \in (-4, 0)$. The method converges for the same interval, since it is consistent.

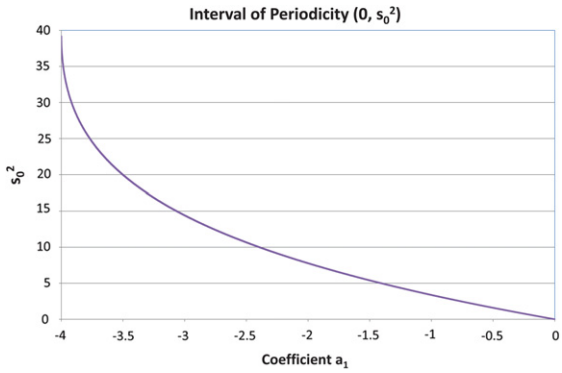

Fig. 1. The interval of periodicity of the new parametric method versus the coefficient a_1.

3.4. Direct relationship between the error and the interval of periodicity

As seen in Fig. 1, the smaller the value of a_1 ($a_1 \to -4^+$), the larger the periodicity interval. However, the same happens to the local truncation error, as we can see from Eq. (15) and particularly from the expression $\frac{16-a_1}{240}$, which takes its maximum value when $a_1 \to -4^+$ and its minimum value when $a_1 \to 0^-$. So the target is to determine the optimal value of a_1 that minimizes the error, while in the same time the method is stable.

4. Application and numerical results

4.1. The problems

4.1.1. The Schrödinger equation—resonance problem

For the integration of problem (1), we consider the case of $E > 0$ over the interval $[0, 15]$ with the boundary conditions $y(0) = y(15) = 0$, using the well known Woods–Saxon potential. The justification is as follows.

As $x \to \infty$, both $V(x)_{x\to\infty} = 0$ and $\frac{l(l+1)}{x^2}_{x\to\infty} = 0$ and the solution of (1) becomes

$$y(x)_{x\to\infty} = P\ \sin\left(k\,x - l\,\frac{\pi}{2} + \delta_l\right), \tag{17}$$

where $k = \sqrt{E}$, $P \in \mathcal{R}$ and δ_l is called *scattering phase shift*.

Usually for $x \gg 0$ (i.e. $x = 15$) the potential decays faster than the centrifugal potential, so $V(x) \ll \frac{l(l+1)}{x^2}$ (asymptotic region), for which case the solution of (1) becomes

$$y(x) \simeq k\,x\,(Q\,j_l(k\,x) - R\,n_l(k\,x)), \tag{18}$$

where j_l and n_l are the *spherical Bessel* and *Neumann* functions and $Q, R \in \mathcal{R}$ [29, pp. 437].

From the comparison of Eqs. (17) and (18), we get:

$$\begin{aligned} Q &= c\ \cos(\delta_l) \\ R &= c\ \sin(\delta_l) \end{aligned} \tag{19}$$

where $c \in \mathcal{R}$ is called *normalization factor*.

Eq. (18) can now take the form

$$y(x) \simeq T\,k\,x\,(j_l(k\,x) - \tan(\delta_l)\,n_l(k\,x)), \quad T \in \mathcal{R}. \tag{20}$$

From Eq. (20) for the discrete points x_a and x_b of the asymptotic region, where $x_a < x_b$, we can derive an approximation of δ_l, which is given by the following expression

$$\tan(\delta_l) \simeq \frac{y(x_a)\,S(x_b) - y(x_b)\,S(x_a)}{y(x_b)\,C(x_a) - y(x_a)\,C(x_b)}, \tag{21}$$

where $S(x) = k\,x\,j_l(k\,x)$ and $C(x) = k\,x\,n_l(k\,x)$.

We consider the case where $l = 0$. Then the above problem and for a chosen value of $\delta_l = \frac{\pi}{2}$ will have a solution only for discrete values of energy E (also called eigenenergies). Here, we use in advance a known eigenenergy $E = 989.701916$, in order to approximate the scattering phase shift δ_l with various numerical algorithms and thus measure their efficiency.

As for the frequency ω, we will use what was suggested in [30] and is given by

$$\omega = \begin{cases} \sqrt{E + 50}, & x \in [0, 6.5] \\ \sqrt{E}, & x \in (6.5, 15]. \end{cases} \tag{22}$$

Table 1
Characteristics of compared methods.

Method	Interval	L.T.E.
Raptis–Allison	$(0, \infty)$	$-\frac{1}{240}(y^{(6)}(x) + y^{(4)}(x)\omega^2)h^6$
Simos–Psihoyios	(0,7.08)	$\frac{1}{2800}(-76\,y^{(5)}(x) - 405\,y^{(4)}(x) + 329\,y^{(3)}(x)\omega^2)h^5$

4.1.2. Inhomogeneous equation

$$y'' = -100\,y + 99\,\sin(t), \qquad y(0) = 1, \qquad y'(0) = 11 \quad t \in [0, 10^4]. \tag{23}$$

Theoretical solution: $y(t) = \sin(t) + \sin(10\,t) + \cos(10\,t)$.
Estimated frequency: $\omega = 10$.

4.1.3. Duffing's problem

$$y'' = -y - y^3 + 0.002\cos(1.01\,t), \qquad y(0) = 0.200426728067, \qquad y'(0) = 0, \tag{24}$$

with $t \in [0, 10^5]$.
Theoretical solution [12]: $y(t) = 0.200179477536\cos(1.01\,t) + 2.46946143 \cdot 10^{-4}\cos(3.03\,t) + 3.04014 \cdot 10^{-7}\cos(5.05\,t) + 3.74 \cdot 10^{-10}\cos(7.07\,t) + \cdots$.
Estimated frequency: $\omega = 1$.

4.1.4. Orbital problem by Stiefel and Bettis

This is an "almost" periodic orbital problem studied by Stiefel and Bettis and can be described by

$$y'' + y = 0.001\,e^{i\,t}, \qquad y(0) = 1, \qquad y'(0) = 0.9995i, \quad y \in \mathcal{C}, \tag{25}$$

or equivalently by

$$\begin{aligned} &u'' + u = 0.001\,\cos(t), \qquad u(0) = 1, \qquad u'(0) = 0, \\ &v'' + v = 0.001\,\sin(t), \qquad v(0) = 0, \qquad v'(0) = 0.9995. \end{aligned} \tag{26}$$

The theoretical solution of problem (25) is given below:

$$\begin{aligned} &y(t) = u(t) + i\,v(t), \quad u, v \in \mathcal{R} \\ &u(t) = \cos(t) + 0.0005\,t\,\sin(t), \\ &v(t) = \sin(t) - 0.0005\,t\,\cos(t). \end{aligned}$$

The system of Eq. (26) has been solved for $t \in [0, 10^5]$.
Estimated frequency: $\omega = 1$.

4.1.5. Nonlinear equation

$$y'' = -100\,y + \sin(y), \qquad y(0) = 0, \qquad y'(0) = 1 \quad t \in [0, 20\,\pi]. \tag{27}$$

The theoretical solution is not known, but we use $y(20\,\pi) = 3.92823991 \cdot 10^{-4}$ [28].
Estimated frequency: $\omega = 10$.

4.2. The methods

In order to determine the efficiency of the new parametric method, we compare it to two well-known optimized methods with variable coefficients of the same order four, while integrating the above problems. All methods tested are listed below:

- The parametric phase-fitted method developed here, for a wide range of values of coefficient a_1.
- The P-stable exponentially-fitted implicit 2-step method developed in [15].
- The exponentially-fitted 3-step predictor–corrector method developed in [11].

At Table 1 we can see the interval of periodicity $(0, s_0^2)$ and the principal term of the local truncation error.

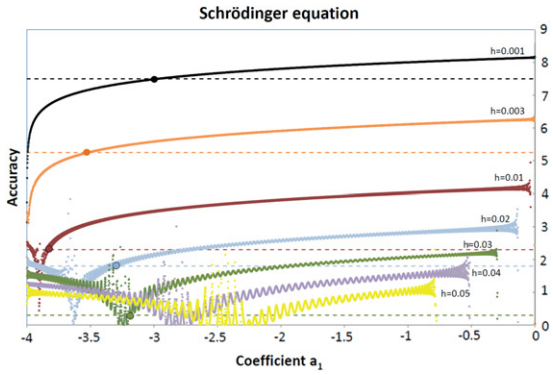

Fig. 2. Accuracy of the new parametric method for the Schrödinger equation. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

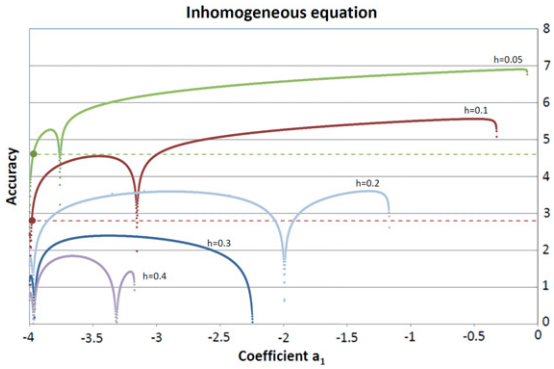

Fig. 3. Accuracy of the new parametric method for the Inhomogeneous equation.

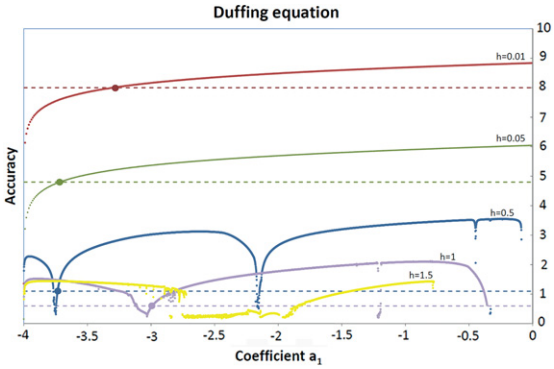

Fig. 4. Accuracy of the new parametric method for Duffing's problem.

4.3. The results

4.3.1. Explanation of the graphs

In Figs. 2–6, we can see the accuracy of the new parametric method, expressed by $-\log_{10}(error)$, versus the value of coefficient a_1. For the cases that the accurate solution of the problem is known, that is for the Inhomogeneous equation, Duffing's problem and the Stiefel–Bettis problem, the *error* is the maximum absolute value of the errors at each integration step. For the Schrödinger equation the error is given by $error = |\delta_l - \pi/2|$. Finally for the Nonlinear equation, for which the theoretical solution is not known, the error is calculated at the end point of the integration interval, by using the reference solution given in 4.1.5.

In these figures we see two types of graphs: small dots (which seem like solid lines due to their density) and dashed lines. Each small dot represents the accuracy of the parametric method for the specific value of coefficient a_1. Different

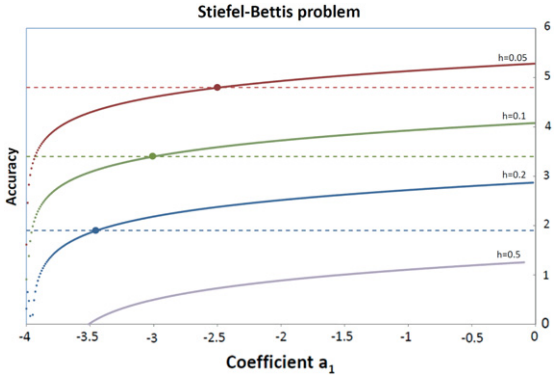

Fig. 5. Accuracy of the new parametric method for the Stiefel–Bettis problem.

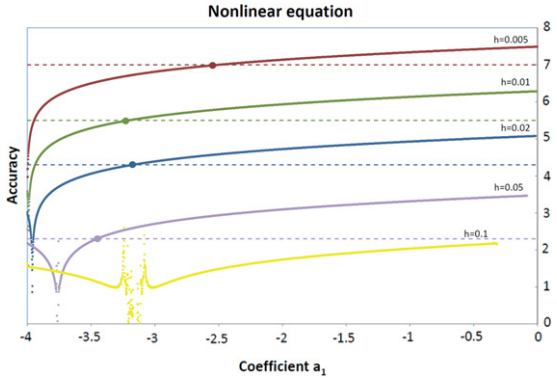

Fig. 6. Accuracy of the new parametric method for the Nonlinear equation.

colors represent different step-lengths of integration used, which can be seen in the legends of the figures. Of course a smaller step-length provides a more accurate solution, thus it exists higher both in the graph and in the legend.

The dashed line (of a specific color) represents the highest accuracy achieved by the other methods under comparison (Section 4.2) that need the same CPU time with the new parametric method for the specific step-length of integration (same color dots).

For example in Fig. 2 the new parametric method for a step-length $h = 0.001$ (black dots) begins with a very low accuracy (<5) for $a_1 \to -4^+$ and ends to a high accuracy (>8) for $a_1 \to 0^-$. The most efficient of the other compared methods that needs the same CPU time as the new method for $h = 0.001$ has accuracy approximately 7.5 and is seen as a black dashed line. Of course the line is horizontal, since the accuracy does not depend on a_1. We add a circle filled with the same color to show the point of intersection. The circle helps us to easily notice that the new parametric method is more accurate than the other methods under comparison for all values of approximately $a_1 > -3$.

In cases where the small dots do not appear in the graph, the parametric method is unstable. This usually happens for large values of step-length h and for large values of coefficient a_1. If a dashed line does not appear, that means that none of the other compared methods is stable. The latter is the case for $h \geqslant 0.04$ for the Schrödinger equation, for $h \geqslant 0.2$ for the Inhomogeneous equation, for $h = 1.5$ for the Duffing equation, for $h = 0.5$ for the Stiefel–Bettis problem and for $h = 0.1$ for the Nonlinear equation.

All numerical computations were carried out on a PC (i7@3.33 GHz) using Matlab 2010 and the CPU time was computed by the built-in function *cputime* for the duration of the actual numerical integration.

4.3.2. *Efficiency of the new method*

First we comment on the efficiency of the new parametric method as compared to the other tested methods. We can observe that there is a large interval in which a_1 lies in, that renders the new method the most accurate. These intervals start from the intersection point of the small dots and the dashed line (denoted with a filled circle). For the Schrödinger equation this is approximately -3, for the Inhomogeneous equation -3.9, for Duffing's problem -3.3, for the Stiefel–Bettis problem -2.5 and for the Nonlinear equation -2.5 (always on the safe side).

As for the right endpoint of the interval, it depends on whether we seek for a solution with a high accuracy or for a fast solution with a low accuracy. In the first case, where the step-length of integration is small and generally s_0^2 lies within the periodicity interval, the parametric method is stable even when $a_1 \to 0^-$, with an exception of Inhomogeneous equation,

Table 2
Minimum and maximum values for a_1.

Problem	min	max (low)	max (high)
Schrödinger	−3.0	−0.8	0.0
Inhomogeneous	−3.9	−3.4	−0.1
Duffing	−3.3	−0.8	0.0
Stiefel–Bettis	−2.5	−0.2	0.0
Nonlinear	−2.5	−0.4	0.0

where $a_1 < -0.1$. We always want to select a value for a_1 as close to the right endpoint of the interval as possible, because of the increased accuracy.

There are some spikes in the accuracy of the new methods for various values of h and a_1. These occur due to the resonances caused by the spurious roots of the characteristic equation of the method, which of course are different for various values of a_1. This is unavoidable for all linear multistep methods with more than two steps. Quinlan has thoroughly investigated this behavior (details can be found in [13]). Fortunately, for the suggested optimal values of a_1, provided in Section 4.3.3, the new method is always more efficient than the compared methods (with an exception of Inhomogeneous equation, where none of the methods is stable).

As we seek for a faster solution with lower accuracy, e.g. 1, we must also lower the right endpoint of the interval that a_1 lies in so that the method is stable. That would be −0.8 for the Schrödinger equation, −3.4 for the Inhomogeneous equation, −0.8 for Duffing's problem, −0.2 for the Stiefel–Bettis problem and −0.4 for the Nonlinear equation. We must note that the very low right endpoint for the Inhomogeneous equation results from the nature of the problem itself. This can be seen from the fact that for a step-length $h \geqslant 0.2$ all other methods under comparison are unstable. All minimum and maximum values for both low and high accurate solutions are presented in Table 2.

4.3.3. Selection of the optimal values of the parameter

Based on the analysis of the previous section, the optimal values for the new parametric method are:

- $\boldsymbol{a_1} = -\frac{1}{10}$, when we need a high accurate solution (>7),
- $\boldsymbol{a_1} = -\mathbf{1}$, when we need a fast low accurate solution (≈ 1) and
- $\boldsymbol{a_1} \in \left(-\mathbf{1}, -\frac{1}{10}\right)$, when we need a medium accurate solution.

5. Conclusions

We developed an efficient parametric symmetric linear phase fitted four-step method for the numerical solution of the Schrödinger equation and related oscillatory problems. We provided the analysis of the local truncation error for the general case and for the Schrödinger equation and the analysis of the periodicity interval. We revealed the direct relationship between the error and the periodicity interval. We also measured the efficiency of the new method for a wide range of possible values of the parameter and made a comparison to other well known methods from the literature. The analysis and the numerical results led us to the optimal values of the parameter, which render the new method highly efficient.

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